

REPORT DOCUMENTATION PAGE					Form Approved OMB No. 0704-0188	
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1. REPORT DATE (DD-MM-YYYY) 06-10-2009		2. REPORT TYPE Final Report		3. DATES COVERED (From - To) 01-09-2007 to 31-08-2009		
4. TITLE AND SUBTITLE STTR (Phase II) - Environmentally-Benign Oxidizers for Propulsion				5a. CONTRACT NUMBER FA9550-07-C-0105		
				5b. GRANT NUMBER FA9550-07-C-0105		
				5c. PROGRAM ELEMENT NUMBER		
6. AUTHOR(S) Karl O. Christe, Ralf Haiges, William W. Wilson, Ross I. Wagner, CJ Jones				5d. PROJECT NUMBER		
				5e. TASK NUMBER		
				5f. WORK UNIT NUMBER		
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Science & Technology Applications, LLC, 301 Science Drive, Suite 210, Moorpark CA 93201				8. PERFORMING ORGANIZATION REPORT NUMBER		
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) Air Force Office of Scientific Research 875 North Randolph Street Suite 325, Room 3112 Arlington, VA 22203				10. SPONSOR/MONITOR'S ACRONYM(S) AFOSR		
				11. SPONSOR/MONITOR'S REPORT NUMBER AFRL-OSR-VA-TR-2013-0993		
12. DISTRIBUTION/AVAILABILITY STATEMENT Distribution A - Approved for public release						
13. SUPPLEMENTARY NOTES						
<div style="border: 1px solid black; padding: 10px; margin: 10px 0;">20130919045</div>						
14. ABSTRACT <p>This program was a Phase II Small Business Technology Transfer Program (STTR) contract with the Air Force Office of Scientific Research (Contract FA9550-07-C-0105). It was carried out by Science & Technology Applications, LLC as the Small Business and the University of Southern California as the Academic Institution. The goal of this proposal was the identification, synthesis and characterization of novel compounds which can serve as a nontoxic replacement for ammonium perchlorate (AP).</p> <p>The program has been highly successful. Two promising target compounds, the ammonium salts of the tetranitroborate and the tetrakis (3,5-dinitro-1,2,4-triazolyl)borate anion, B(DNT)4-, were identified as excellent candidates for replacing AP. Umpolung reactions were studied as a possible synthetic route towards the tetranitroborate anion, several suitable B(NX)4- skeletons were synthesized and characterized. The most impressive progress was made in the area of B(DNT)4- chemistry. The B(DNT)4- anion was successfully synthesized and characterized. It has good thermal stability, is hydrolytically stable, is insensitive, and the predicted performance of its ammonium salt is slightly higher than that of AP.</p>						
15. SUBJECT TERMS <p>Ammonium perchlorate, tetranitroborate anion, tetrakis(3,5-dinitro-1,2,4-triazolyl)borate anion,</p>						
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON	
a. REPORT	b. ABSTRACT	c. THIS PAGE			Karl O. Christe	
Unclassified	Unclassified	Unclassified	UU	21	19b. TELEPHONE NUMBER (Include area code) 213-740 3552	



Progress Report

Contract No: FA9550-07-C-0105

Phase II STTR: Environmentally Benign Ox for Propulsion
Progress Report: 30 Nov 2007

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Programmatic

1. AFOSR Program Manager is Dr. Michael Berman.
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703.696.7781
2. CLIN 000101 for a total of \$ \$374,859 has been obligated.
3. POP is 01 Sep 07 – 31 Aug 08.
4. STA has registered in WAWF system.
5. Preliminary Authority to Proceed issued to USC in Oct 07. Final contract expected to be issued by Dec 07.

Technical for CLIN 000101

1. Two papers on the energetics of decomposition of CF_3OH and on CHFO and related compounds were written and accepted by Inorg. Chem. for publication.
2. In collaboration with Dave Dixon, a manuscript was written on the calculation of reliable bond energies in period 2 fluorides and oxofluorides, demonstrating the great impact which reorganization energies have on the adiabatic and diabatic dissociation energies. The paper was submitted to the Journal of Physical Chemistry and accepted for publication.
3. Three manuscripts were reviewed for different journals.
4. A draft for a manuscript on the isomerization equilibria of N_2F_2 was written. Numerous experiments need to be repeated to clarify discrepancies in the original data.

Published Documents

Theses:

Joshua Saul Wittenberg, "The Behavior of Semiconductor Nanocrystals Under Intense Ultraviolet Irradiation and Shock Wave Compression," UC Berkeley Department of Chemistry Doctoral Thesis, (December, 2008).

Noelle Marie Drugan Kamp, "Probing the Internal Environment of Hollow Metal Oxide Nanoparticles," UC Berkeley Department of Chemistry Doctoral Thesis, (May, 2009).

Papers published:

Park, J.; Zheng, H.; Jun, Y.; Alivisatos, A. P.; **Hetero-epitaxial anion exchange yields single-crystalline hollow nanoparticles.** *J. Am. Chem. Soc.* **2009**, 131, 13943-13945.

Wittenberg, J.S.; Merkle, M.G.; Alivisatos, A.P.; **Wurtzite to Rocksalt Phase Transformation of Cadmium Selenide Nanocrystals via Laser-Induced Shock Waves: Transition from Single to Multiple Nucleation.** *Phys. Rev. Lett.* **2009**, 103, 125701.

Cabot, A.; Smith, R. K.; Yin, Y.; Zheng, H.; Reinhard, B. M.; Liu, H.; Alivisatos, A. P. **Sulfidation of Cadmium at the Nanoscale.** *ACS Nano* ; **2008**, 2(7), 1452-1458.